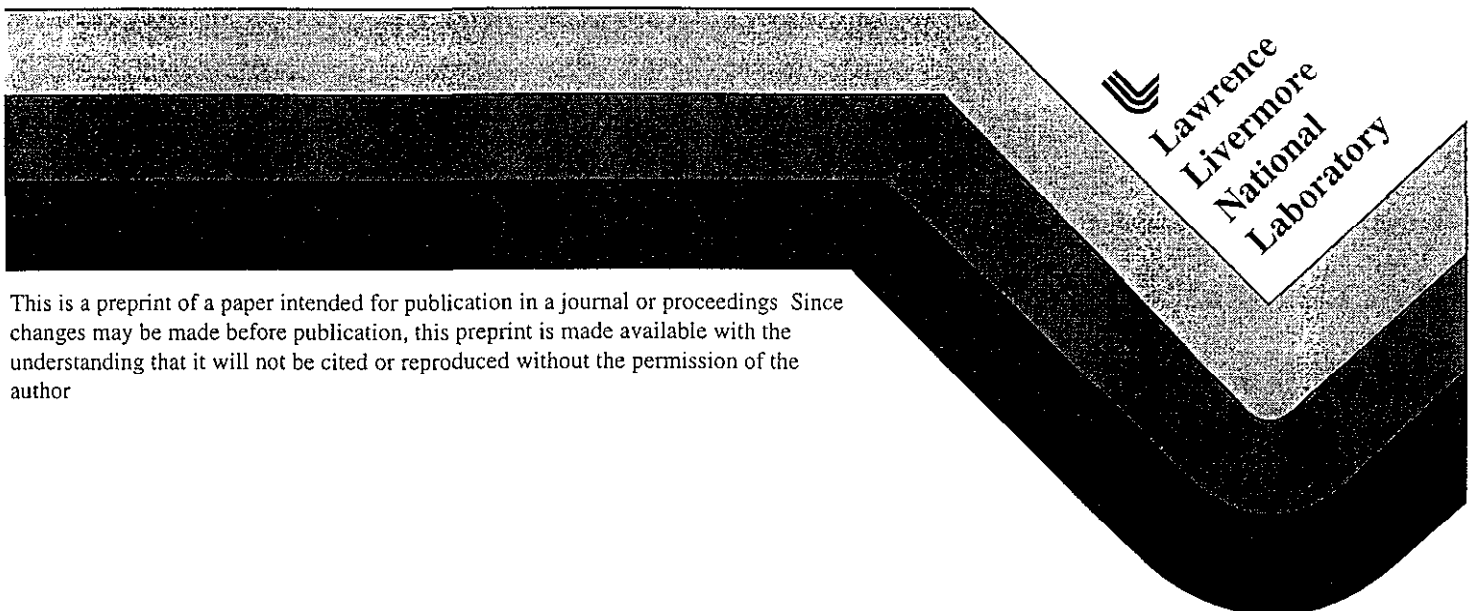# Kinetic Information from Detonation Front Curvature

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KINETIC INFORMATION FROM DETONATION FRONT CURVATURE

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The time constants for time-dependent modeling may be estimated from reaction zone lengths, which are obtained from two sources One is detonation front curvature, where the edge lag is close to being a direct measure The other is the Size Effect, where the detonation velocity decreases with decreasing radius as energy is lost to the cylinder edge A simple theory that interlocks the two effects is given A differential equation for energy flow in the front is used, the front is described by quadratic and sixth-power radius terms The quadratic curvature comes from a constant power source of energy moving sideways to the walls Near the walls, the this energy rises to the total energy of detonation and produces the sixth-power term The presence of defects acting on a short reaction zone can eliminate the quadratic part while leaving the wall portion of the curvature A collection of TNT data shows that the reaction zone increases with both the radius and the void fraction

QUADRATIC CURVATURES

New kinetic, ie time-dependent, explosive models need input data, and a first cut may be had by obtaining reaction zone lengths for promptly detonating explosives at steady state, ie with constant two-dimensional confinement effects Direct measurements of these reaction zones have not been made, so that any approach will necessarily be indirect

Detonation front curvatures of cylinders offer a starting point, and most measured curvatures are of the "quadratic" type as illustrated by J Lee's ANFO data in Figure 1 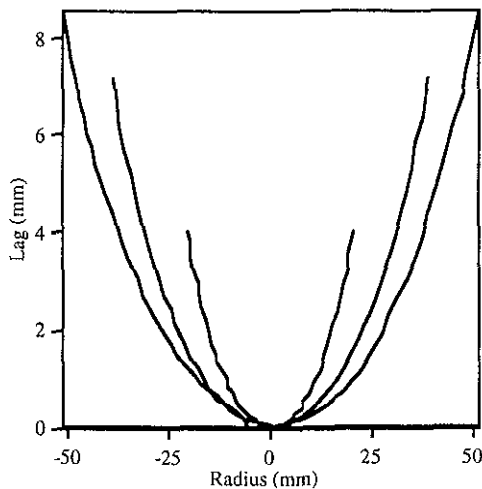[1] The curves are smooth, roughly quadratic and show an edge lag that increases with increasing radius The curves are not truly quadratic but may be described by the function[2]

$$L = AR^2 + BR^6 \tag{1}$$

where L is the detonation lag and R is the radius A and B are constants for a given radius but are variable for different radii The A-term may be thought of as describing the continuous flow of energy from the cylinder axis outward to support the edges The B-term represents the break-out of the wall and shows more scatter in the fitted data The A-term contributes about 50% of the edge lag for small reaction-zone explosives and perhaps 70% for large ones, with there being wide scatter The "average" position for Eq 1 occurs at about $R_o/2^{1/2}$

Figure 2 shows shows a schematic of the reaction zones, both sonic and percent chemical reaction The explosive tries to minimize both the lag and the sonic reaction zone, which suggests the approximation that[2]

$$<x_c> \sim L_o \tag{2}$$

where $<x_c>$ is the average sonic reaction zone length and L_o the edge lag

FIGURE 1 Three radii of unconfined ANFO cylinders fires by J Lee These are of the smooth "quadratic" type The detonation is proceeding downward
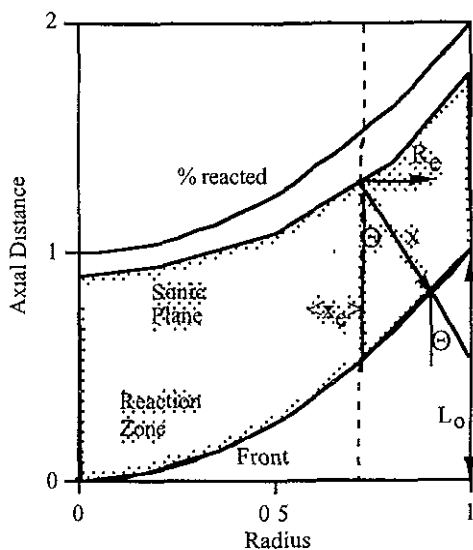
FIGURE 2 Schematic view of the sonic reaction zone for a "quadratic" curvature Θ is the angle of the front at radius R, $<x_e>$ is the average sonic reaction zone length A chemical reaction zone is also shown Detonation is downward

The angle normal to the front at radius R is given by the derivitive

$$\Theta = \tan^{-1}(2AR + 6BR^5) \qquad (3)$$

One test of Eq 3 is the measurement of the edge angle at R_o, which will be 0° for a flat front and larger as the curvature increases Table 1 lists the measured and calculated edge angles taken only from high quality runs where digital files are available [3-7] The radius of curvature, which varies with radius, is

$$R_{cur} = R/\sin\Theta \qquad (4)$$

Considerable error exists in determining the experimental angles The various families of explosives show the same measured edge angle within error The addition of metal containment, seen with the PBXN-111, reduces both the lag and the angle An exceptionally large angle appears in the PBX-9502 data

TABLE 1 Measured and calculated edge angles for assorted explosives PETN and LX-14 are not quadratic

| | Degrees | | Measd |
	Meas	Calc	Stdev
PETN	3	3	
LX-14	4	5	
QM100R	12	9	5
LX-04	14	9	9
PBXN-111- N Con	16	16	8
PBXN-111- A Con	17	15	7
Ultrafine TATB	18	14	3
NM ANFO	20	26	5
PBXN-111-N Unc	26	30	10
HANFO	26	36	11
PBXN-111-A Unc	33	31	18
PBX-9502	39	22	16

The Size Effect theory for a cylinder was constructed with the relations[8]

$$\left(\frac{<E_o>}{E_o}\right)^{1/2} = \frac{U_s}{D} = 1 - \frac{R_e}{R_o}$$

$$= 1 - \frac{<x_e>}{\sigma R_o} \qquad (5)$$

where $<E_o>$ and U_s, E_o and D are the total detonation energies and velocities in cylinders of radius R_o and infinite size, respectively "Infinite" radius also means radius R_o with perfect wall confinement R_e is the thickness of the skin layer on the edge that loses all energy and requires energy replacement from the interior σ is a function that relates R_e and the reaction zone length Eq 5 is a relation between cylindrical volumes, chemical energy density and detonation velocity

It would be useful to relate curvature with the Size Effect, where the detonation velocity changes with radius In Figure 2, at the average radius $<R> = 0\ 707R_o$, we define the average angle of the front $<\Theta>$ and write

$$<x_e> \approx \frac{R_o(1 - U_s/D)}{\sin<\Theta>\cos<\Theta>} \qquad (6)$$

where we assume that the sideways distance for energy to be shipped is equal to the skin layer thickness, R_e

From Eqs 5 and 6, we see that

$$\sigma = [\sin<\Theta>\cos<\Theta>]^{-1} \qquad (7)$$

The result of this approach is that the equality of reaction zone length and edge lag given in Eq 2 is only approximately true We find, for the TATB, PBXN-111 and ANFO groups, an average ratio of

$$<x_e>/L_o \sim 2 3 \pm 1 6 \qquad (8)$$

SIMPLE DERIVATION

The "quadratic" shape arises because the explosive moves energy sideways to shore up the moving wall We use the mathematics for calculation of temperature in a cylinder with internal heat generation [9] The lag, L, may be described by [28]

$$\nabla^2 L = \frac{1}{R}\frac{\partial}{\partial R}\left(R\frac{\partial L}{\partial R}\right) = \frac{A_o}{K} = 4A + 36BR^4 \qquad (9)$$

where R is the radius, A_o is the sideways power and K is the energy conductivity

We can calculate the A term by assuming that all of the constant sideways quadratic energy is given by $E_o - <E_o>$, which, from Eq 5, is

$$E_o - <E_o> = \beta\left[1 - \left(1 - \frac{<x_e>}{\sigma R_o}\right)^2\right]E_o$$
$$\approx \frac{2\beta<x_e>E_o}{\sigma R_o} \qquad (10)$$

Above, βE_o is the total actual energy of detonation obtained within the reaction zone, so that E_o is reserved for the total energy calcuated from the thermochemical code For most homogeneous and heterogeneous explosives, we expect β to be 1, but for composites, it may be much smaller For PBXN-111, for example, the aluminum and AP probably do not react within the reaction zone, so that $\beta E_o \approx 2$-4 kJ/cc whereas the complete reaction produces 13 kJ/cc

The power in Eq 9 is the energy divided by time, which is $1/U_s$ across 1 cm We divide by K and compare with 4A from Eq 9

$$A = \left(\beta\frac{U_s E_o}{K}\right)\frac{<x_e>}{2\sigma R_o} \qquad (11)$$

A is obtained from the curvature, so that we get the energy conductivity from

$$K = \frac{\beta E_o U_s}{A}\left(\frac{<x_e>}{2\sigma R_o}\right) \qquad (12)$$

For TATB explosives, $K \sim 90 \pm 50$ MW/mm^2 For PBXN-111 and ANFO $K \sim 90 \pm 4$ and 300 ± 220 MW/mm^2 Overall, K is roughly 100 MW/mm^2 We have no similiar treatment for B

The energy density of an imaginary 1 cc cube may be converted to total energy, differentiated and adjusted for the side surface area to give the pressure on the front

$$P = P_o - \frac{K}{U_s}(4A + 36BR^4)$$
$$= P_{max} - \frac{K}{U_s}36BR^4 \qquad (13)$$

The pressure is expected to decrease more steeply than the curvature increased For TATB explosives, we find the maximum B term to amount to 0 GPa for $R_o = 25$ mm but 4-11 GPa for $R_o = 5$-6 mm

For the Wood-Kirkwood 1 1/2-dimensional analytical model that describes a single cell on the axis of a cylinder,[10] we define a radius of curvature of the detonation front

$$R_{cur} \sim R/(2AR + 6BR^5) \longrightarrow 1/2A \text{ for } R \longrightarrow 0 \quad (14)$$

Using the equations above, the radial particle velocity in the model is

$$u_r = \frac{P \tan\Theta}{\rho_o U_s} = \frac{1}{\rho_o U_s}\left(P_o - \frac{K}{U_s}4A\right.$$
$$\left. - \frac{K}{U_s}36BR^4)(2AR + 6BR^5\right) \quad (15)$$

and the radial W-K function becomes

$$\frac{\partial u_r}{\partial R} = \omega_r = \frac{2A}{\rho_o U_s}\left(P_o - \frac{K}{U_s}4A\right)$$
$$= \frac{2AP(\text{axis})}{\rho_o U_s} = \frac{u_p}{R_{cur}} \quad (16)$$

It would be useful to obtain an on-axis radius of curvature from the Size Effect data Using Eq 7, we can calculate from σ to $<\Theta>$ by iteration Unfortunately, $<\Theta>$ contains elements of B as well as A, so that on-axis behavior for curvatures is given to $\pm15\%$ by

$$R_{cur}(\text{on-axis}) = \frac{1}{2A} \approx \frac{R_o}{\tan<\Theta>} \quad (17)$$

This is used to calculate R_{cur} from the Size Effect data

NON-QUADRATIC CURVES

A second type of non-quadratic curvature is found for explosives with small reaction zones , as seen for 1 82 g/cc LX-14 (95 5% HMX, 4 5% estane) in Figure 3 [3] The center is ragged and turbulent and often contains a "sombrero" perhaps caused by non-parallel cylinder faces Excluding the center, the curve may be fit to

$$L = BR^6 \quad (18)$$

so that only the wall term is present We postulate that defects such as inert grains or large voids scatter the front, and only the energy from the outermost regions flows to the edges The curve is symmetric because the defect size
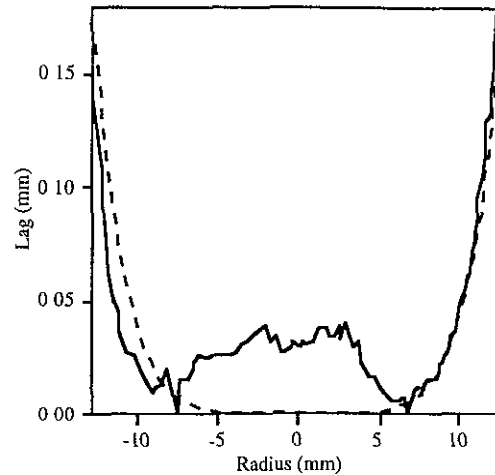

FIGURE 3 Detonation front curvature of non-quadratic LX-14 taken with a 7500 rpm rotor and a writing speed of 30 mm/μs The dashed line fits BR^6 A tilt correction to the data has been made

is much smaller than the cylinder radius

Another non-quadratic case appears when the defect size is about 1/10 the radius and extreme disruption of the front occurs Figure 4 shows two shots with the paste explosive RX-08-HD (74% HMX, 20 TMETN, 6 urethane binder) [3] The upper one is defect-free and shows a quadratic shape The lower had mm-sized holes as seen by x-rays The center is massively disrupted, yet the edge lags are still visible 1 1 mm for the top and 0 4 - 0 6 mm at the bottom, suggesting that the holes cut the reaction zone length in half The detonation velocites were 8 15 and 8 04 mm/μs, showing that the defects do indeed slow the speed

THE SIZE EFFECT

We return to further consider the Size Effect and see if we can get more data to use We use Eq 7 to calculate σ for the curvature samples with TATB, PBXN-111, ANFO

and other individual samples where D can be extrapolated with some confidence The results are plotted in Figure 5 vs $1 - U_s/D$ and the fitted curve is

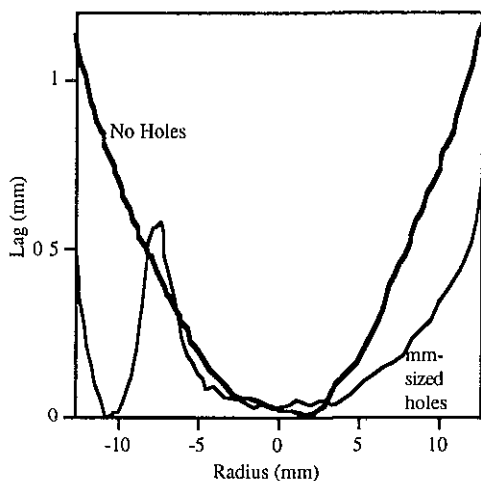$$\sigma \approx \frac{2\ 2}{(1 - U_s/D)^{1/3}}$$

(19)

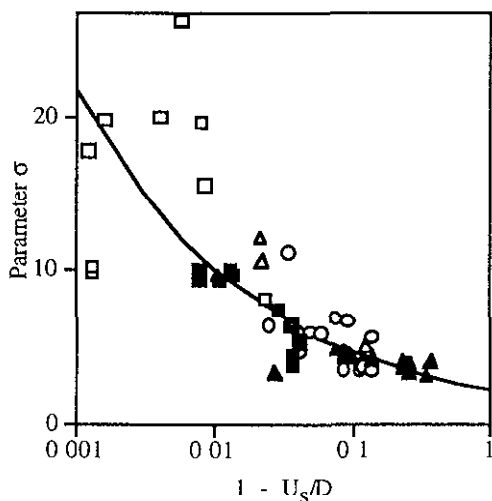**FIGURE 4** Effects of holes in distorting the detonation front of the paste explosive RX-08-HD

FIGURE 5 Calibrating the σ function with curvature data The data includes all types of explosives where D can be reasonably extrapolated

Using this, we may take all the Size Effect data that exists and calculate the Size Effect reaction zone lengths from Eq 5

$$\langle x_e \rangle = \sigma R_o \left(1 - \frac{U_s}{D} \right)$$

(20)

CONVERTING TO KINETICS

We next want to convert our results to obtain the time constant, τ, where the simplest burn relation might be

$$\frac{dF}{dt} = G\,\frac{P^2(1 - F)}{\tau}$$

(21)

where F is the fraction burned, P the pressure and G the rate constant The best that we can do is assume the same number of time constants, $n \sim 5$, in the burn of every explosive Many (but not all) samples follow this empirical relation

$$\langle x_e \rangle / R_o^{1/2} \sim \text{constant}$$

(22)

This allows us to calculate $\langle x_e \rangle$ for a constant set of radii, a possibly unnecessary refinement The rate constant for Eq 21 is roughly

$$G \approx \frac{5U_s}{\langle x_e \rangle\,(5P_{cj}/4)^2}$$

(23)

where the thermochemcial C-J pressure is multiplied by 5/4 to approximate the spike pressure Table 2 shows a comparative list of rate constants that might be used as input to a kinetic code

DISCUSSION

The reaction zone lengths have been derived using a circular model and are good to perhaps ±100% Only direct measurement with gauges will fix the numbers, and we might expect them to all move in proportion We next consider the broad TNT data set of Stesik and Akimova [11]

TABLE 2 Table of comparative rates obtained from Size Effect data for a 12 7 mm radius Five time constants inside the reaction length are used.

	$<x_e>$ (mm)	G (μs^{-1*} GPa^{-2})
TNT 1 62 g/cc	1 4	0 04
PBX-9404	0 6	0 04
TNT 1 0 g/cc	6 5	0 045
PBX-9501	0 6	0 04
Comp B	0 9	0 04
ANFO SW	8	0 02
ANFO 0 95 g/cc	11	0 022
PBX-9502	2 3	0 014

Figure 6 shows the calculated ratio $<x_e>/R_o^{1/2}$ plotted a s a function of void volume, f_v, for cylinders of various radii The void volume is calculated from
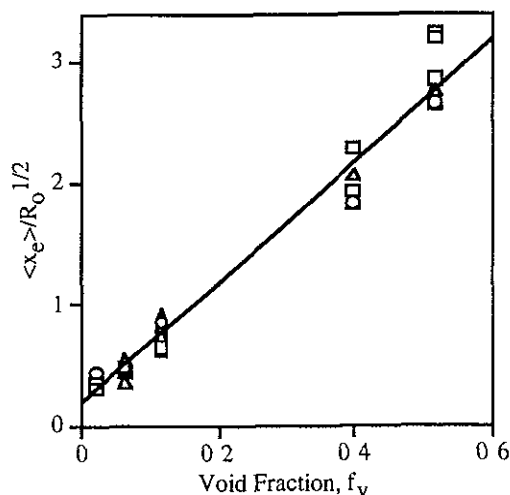
$$f_v = 1 - \rho_o/\rho(TMD) \qquad (24)$$

FIGURE 6. Reaction zone length for cylinders of fixed radius for TNT [13] Void space increases the reaction zone The circles are 15-16 mm radii, squares are for 4-5 mm, the rest from 1 6-20 mm are triangles

The data in Figure 6 may be fit by the empirical equation

$$<x_e>/R_o^{1/2} \sim 0 18 + 5 0f_v \qquad (25)$$

The $R_o^{1/2}$ term removes the dependence of the radius for these samples The reaction zone increases with increasing void fraction but by much more than might be expected If only the void volume were added directly to the reaction zone volume, we would expect

$$<x_e>/R_o^{1/2} \sim 0 18 + 0 36f_v \qquad (26)$$

Does the approach of Eq 25 work for the other Size Effect data? The results are shown in Figure 7 The fast group of explosives includes PETN, RDX, HMX, ADNBF, DNBF and "pure" TNT Some explosives with a few percent binder are included The slow group includes "impure TNT" (Figure 6), tetryl, DNT, EDNA, picric acid, TATB, NTO, DINGU and RDX/polyethylene wax The general appearance of the figure is the same
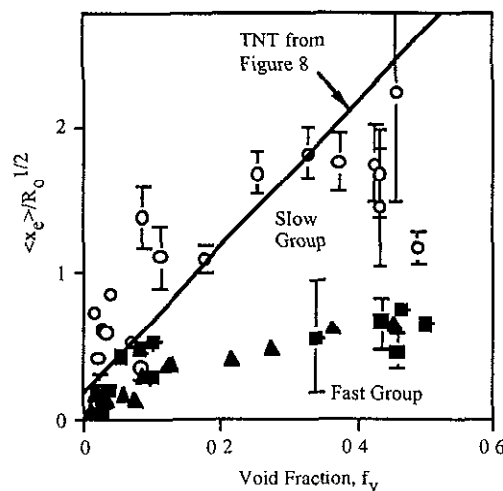

FIGURE 7 Addition of more Size Effect data to the TNT line of Figure 6 A slow and a fast group of explosives are defined

SUMMARY DATA

A collection of detonation front curvature and Size Effect data is available in P C Souers, "A Library of Prompt Detonation Reaction Zone Data," Lawrence Livermore Laboratory UCRL-ID-130055 (1998)

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